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Title: Multi-scale Pore-network Representation of Heterogeneous Carbonate Rocks

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Key points:

- This work investigates the multi-scale porosity of a carbonate rock.
- We explore representativeness of multi-scale networks by comparing simulated and laboratory measured capillary-pressure vs saturation curves.
- We present a workflow for selecting number and length scales of networks to generate multi-scale pore-networks.

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## Abstract:

A multi-scale network integration approach introduced by *Jiang et al.* [2013] is used to generate a representative pore-network for a carbonate rock with a pore-size distribution across several orders of magnitude. We predict the macroscopic flow parameters of the rock utilising i) 3D images captured by X-ray computed micro-tomography and ii) pore-network flow simulations. To capture the multi-scale pore-size distribution of the rock we imaged four different rock samples at different resolutions and integrated the data to produce a pore-network model that combines information at several length-scales that cannot be recovered from a single tomographic image. A workflow for selection of the number and length-scale of the required input networks for the network integration process, as well as fine tuning the model parameters is presented. Mercury injection capillary-pressure data were used to evaluate independently the multi-scale networks. We explore single-scale, two-scale, and three-scale network models and discuss their representativeness by comparing simulated capillary-pressure versus saturation curves with laboratory measurements. We demonstrate that for carbonate rocks with wide pore-size distributions, it may be required to integrate networks extracted from two or three discrete tomographic data sets in order to simulate macroscopic flow parameters.

## 1. Introduction

Pore-scale fluid flow simulation is a useful tool for calculation of the macroscopic transport properties of porous media, specifically for homogeneous systems [*Meakin and Tartakovsky*, 2009; *Joekar-Niasar and Hassanizadeh*, 2012; *Blunt et al.*, 2013; *Wildenschild and Sheppard*, 2013]. For complex porous material realistic representation of the pore structure is essential for successful simulations but has proven to be challenging. High-resolution X-ray computed micro-tomography ( $\mu$ CT) imaging allows detailed study of porous media in 3D (reviews by *Wildenschild and Sheppard* [2013], *Fusseis et al.* [2014], and *Bultreys et al.* [2016]). Reliable application of this technique requires sufficient image quality to allow discrimination of the important features of the sample. Pore-network models (PNM) extracted from binarised  $\mu$ CT images (see review by *Dong* [2007]) are simple representations of pore

structures to simulate flow at a reduced computational cost. Although appealing, PNM predictions often do not agree well with the corresponding laboratory measurements, specifically for complex pore systems such as carbonate rocks [Sorbie and Skauge, 2012]. The trade-off between the sample size and  $\mu$ CT image resolution means that a single  $\mu$ CT volume may not capture the details of a multi-scale pore structure [Hebert *et al.*, 2014]. Capturing a representative image of heterogeneous samples with pore-size distribution (PSD) spanning several orders of magnitude is an outstanding challenge with existing  $\mu$ CT instrumentation. A representative elementary volume (REV) is required that is the smallest sample to which measured properties of the bulk sample can be assigned [Bear, 1972]. Generating two-scale PNM that are representative of complex pore systems has been studied by Biswal *et al.* [2007]; Biswal *et al.* [2009] and Ghous *et al.* [2008], and more recently by Prodanović *et al.* [2015], Mehmani and Prodanović [2014], and Bultreys *et al.* [2015]. Jiang *et al.* [2013] introduced a network integration method to generate PNMs of arbitrarily large volumes that can incorporate multi-scale pore systems extracted [Jiang *et al.*, 2007] from images captured at different resolutions. A detailed PNM extracted from a high resolution  $\mu$ CT volume (fine-network) is combined with a network extracted from a coarse resolution volume (coarse-network). For details of how the nodes/bonds of the differently scaled models are interconnected see Jiang *et al.* [2013]. The domain of the fine-network is smaller than that of the coarse-network, hence a larger network that is statistically equivalent to the fine-network is generated and then integrated into the coarse-network. The generated multi-scale networks can be heavier than the original fine-network, with an adverse effect on the computational cost of fluid flow simulations. To address this Jiang *et al.* [2013], reduced the number of fine-network elements by a fraction ( $f_F$ ) such that  $0 < f_F \leq 1$ . It is also possible to scale the size of the domain of the two-scale network (nesting-domain) with respect to that of

the original coarse image using a scaling factor ( $\delta$ ) that is arbitrary but is restricted by the available computational power for flow simulations.

We investigate generation of a representative PNM for a dolomite using *Jiang et al.* [2013]’s approach and a quasi-static pore-network flow simulator [*Ryazanov et al.* [2009]]. We evaluate *Jiang et al.* [2013]’s approach by comparing simulated  $P_c(S)$  curves with those measured experimentally using mercury injection capillary-pressure (MICP) tests. A workflow is proposed for multi-scale network generation to address (i) the choice of sample size and, hence, image resolution, and (ii) the tuning of model parameters to reproduce the laboratory  $P_c(S)$  curves.

## 2. Imaging and Mercury Porosimetry

A sucrosic dolomite (Silurian Dolomite (SD), Thornton formation, Chicago, Illinois, US) with pore sizes spanning 3 orders of magnitude was used (Figure 1). Laboratory measurements of a 38mm diameter core displayed porosity and permeability of 17% and ~50mD, respectively (Figure 1b).

We imaged, using  $\mu$ CT, four samples of diameter  $D=2, 5, 25$  and 38mm, at resolutions of 2.3, 12, 21 and 32.8 $\mu$ m, respectively (Figure 1b). Both the image voxel sizes and the corrected image resolutions are reported in Table 1, the correction accounts for the unsharpness caused by the X-ray source spot size [*Feser et al.*, 2008]. The values presented throughout the rest of the manuscript are the corrected image resolution values. As currently worded, this is still a bit unclear. Methods are detailed in the SI and *Pak et al.* [2013]. Sizes were selected because 38mm is a standard petrophysical plug, 25mm is the largest sample the MICP could analyse, and 5mm and 2mm provide details of the finer porosity. Figure 1c displays the PSD derived from these four data volumes (Figure 1b) using a sphere fitting method [*Jiang et al.*, 2007]. Each volume has captured only a portion of the PSD. In SD recrystallization to dolomite has produced a structure in which the pores are lined by the apices and edges of dolomite rhombs

with well sorted crystals sizes. Microscope images (Figure S1.) show that smaller pores are formed in between a few crystals, are uniformly present throughout the sample, suggesting little or no spatial correlation of the micro-porosity. Hence, we uniformly integrate the fine-network in the entire nesting-domain.

MICP measurement was performed on three 25 mm diameter SD core plugs imaged at resolution 21 $\mu$ m (Figure S2). MICP provides  $P_c(S)$  curves from which pore-throat size distribution can be extracted [Ritter and Drake, 1945]. The MICP-based porosity for these samples is 18.03, 16.03 and 18.1%. The image-based porosities at this resolution are 8.05, 6.03 and 8.12%, respectively, hence the 21 $\mu$ m represent a coarse-scale resolution.

### 3. Multi-scale PNM Reconstruction

We explore representing the SD pore structure using multi-scale networks to incorporate features extracted from the four  $\mu$ CT volumes shown in Figure 1b. For 3D renderings of these networks see Figure S3. The physical size of these networks can be found from the image dimensions and voxel resolutions (Table 1). The two coarse-scale networks are globally disconnected while the fine-scale networks are connected with simulated absolute permeability  $k_{abs} > 0$  mD. The total (and connected) porosity shows an increasing trend with resolution enhancement, as does the calculated permeability. The two fine-networks display calculated permeability values higher than the laboratory measurement i.e. 50 mD. The small samples do not contain a REV and the calculated permeability values reflect the local connectivity of the pore system at these scales. However, even for the  $2.3\mu\text{m}$  resolution network about 11% of the pore volume is disconnected, reflecting that the resolution is insufficient to capture the smallest pore-throats, or that isolated pores exist in the sample.

#### 3.1. Two-scale PNMs

Six possible combinations for generating two-scale networks are  $32.8\text{-}21\mu\text{m}$ ,  $32.8\text{-}12\mu\text{m}$ ,  $32.8\text{-}2.3\mu\text{m}$ ,  $21\text{-}12\mu\text{m}$ ,  $21\text{-}2.3\mu\text{m}$ , and  $12\text{-}2.3\mu\text{m}$ , referring to image resolution. Essentially, we need (i) a sufficiently large coarse-network that represents the largest pores, (ii) a fine-network with sufficient resolution that captures the smaller pores, and (iii) a sufficient overlap of the PSD of the two networks to ensure representation of the intermediate-size pores. Hence,  $12\text{-}2.3\mu\text{m}$  and  $32.8\text{-}21\mu\text{m}$  combinations are not acceptable. In what follows other combination are discussed.

##### 3.1.1. Combination of 21 and $2.3\mu\text{m}$ PNMs

Figure 2a shows ten networks extracted from sub-domains ( $\delta=0.1\text{-}1$ ) of the  $21\mu\text{m}$  coarse-network. At  $\delta=0.4$  the domain is sufficiently large to accommodate a cluster of large pores,

hence the network porosity displays a sharp increase, Figure 2b. At  $\delta=0.5$  the domain accommodates a connected cluster of pores, therefore,  $k_{abs}>0$ . However, as the sub-domain grows ( $\delta>0.5$ ) the networks become again disconnected, suggesting that only a locally connected cluster is captured at  $\delta=0.5$  which is not representative of the connectivity of larger pores at this scale.

Figure 2c displays the sensitivity of these two-scale networks to  $f_F$ . Porosity increases linearly with the inclusion of increasing fractions of the fine-network, while the permeability starts to converge for  $f_F>0.05$ . Thus even a reduced version of a fine-network can provide the required connectivity to two-scale network.

The calculated porosity and permeability display convergence at  $\delta>0.6$  (i.e. total porosity  $\sim 6\%$  and  $k_{abs}=0$ ). Figure 2d, however, shows that the  $P_c(S)$  curves, calculated using these two-scale PNMs ( $f_F=0.01$ ,  $0.6<\delta<1$ ), do not converge. The curves display jumps at different saturations depending on the nesting-domain size. Examination of Figure 2a reveals that the coarse-network contains two connected clusters of elements (pores and nodes) that are disconnected from each other. Network integration provides connectivity between these clusters through elements of the fine-network. Cluster 1 is connected to the inlet and can be invaded by the injected phase directly. Cluster 2 is only accessible through cluster 1 using the fine-network connections. The jump occurs at saturation  $S^*$  that is equal to the ratio of the volume of cluster 1 to the total volume of the connected pore space.

As  $\delta$  increases, cluster 2 grows more significantly compared to cluster 1, hence  $S^*$  approaches 0.8. Hence, the selected domain from the  $21\mu\text{m}$  resolution image does not contain a REV. However, the MICP core plugs were approximately 60% larger than the box selected for pore-network simulations, and the MICP-driven  $P_c(S)$  curves for three 25mm diameter SD plugs are very close (Figure S2a), this suggests that the MICP plugs themselves are representative for this rock.



### 3.1.2. Combination of 32.8 and 2.3 $\mu$ m PNMs

For this combination the two-scale network porosity converges for  $\delta > 0.6$  (Figure 3a) while  $k_{abs}=0$  for all sub-domains. Further, the simulated  $P_c(S)$  curves for this combination ( $f_F=0.01$ ) also converge for  $\delta > 0.6$  (Figure 3b). This indicates that sub-domains of the 38.2 $\mu$ m image with  $\delta > 0.6$  contain a REV of SD. The  $P_c(S)$  curves, however, show a jump at  $S_{air} \sim 0.8$  causing an overestimation of the experimental capillary-pressure values for  $S_{air} < 0.8$ . The PSD of the 2.3 $\mu$ m network (Figure 1b) shows a peak at  $\sim 6\mu$ m, while pores larger than 10 $\mu$ m display less than 20% probability (i.e. volume fraction). Since the coarse-network is globally disconnected, the two-scale networks are connected only through fine-network elements. The initial displacement ( $S_{air} > 0.8$ ) corresponds to the pores accessible from the inlet. At  $S_{air} \sim 0.8$  the pressure needs to increase sufficiently before elements from the fine-network can be invaded. For the converged set of  $P_c(S)$  curves, on Figure 3b, the  $f_F$  is equal to 0.01. Including a larger  $f_F$  suppresses the jump in the capillary-pressure curve but does not totally remove it. The  $P_c(S)$  curve for the  $\delta=0.6$  and  $f_F=0.04$  network shows a small jump at  $S_{air}=0.8$  from  $\sim 21kP$  to  $\sim 47kP$  corresponding to invasion of pore-throats with radius of 40 $\mu$ m to 16 $\mu$ m. However, this size range is insufficiently represented in both 32.8 and 2.3 $\mu$ m networks. In particular, a small  $f_F$  makes a reduced network less representative of the two ends of the PSD. In practice, the difference in the domain sizes of the coarse and fine-networks causes higher  $f_F$  values to make the two-scale network substantially more computationally expensive.

### 3.1.3. Combination of 32.8 and 12 $\mu$ m PNMs

For this combination the calculated  $P_c(S)$  curves show a good match with the laboratory measurements at  $S_{air} > 0.04$  (Figure 4). However, the simulations stop at capillary-pressure values around 276kP, due to fine-network resolution limitations. Using a higher resolution

fine-network may not provide significant additional connectivity, but may prove essential for calculation of saturation values.

### 3.2. Three-scale PNMs

We have demonstrated that a finer length-scale needs to be integrated into the 32.8–12 $\mu\text{m}$  combination, or an intermediate length-scale must be added to the 32.8–2.3 $\mu\text{m}$  combination.

To integrate three PNMs of different length-scales first the two smaller networks are integrated into a two-scale network that is subsequently integrated into the largest scale network. This involves selecting two sets of  $\delta$  and  $f_F$ . As the number of length-scales increases, sensitivity analysis on the effect of  $\delta$  and  $f_F$  becomes increasingly time consuming.

Figure 5 compares the closest simulated three-scale network  $P_c(S)$  curve with the laboratory measurement. This three-scale PNM is generated by integration of the 2.3 and 12 $\mu\text{m}$  networks ( $\delta=1, f_F=0.004$ ) followed by integration of that network with the 32.8 $\mu\text{m}$  network ( $\delta=0.7, f_F=0.006$ ). The nesting-domain sizes for the 2.3 and 12 $\mu\text{m}$  networks are close, hence selecting  $\delta=1$  is feasible. To keep the three-scale network computationally manageable while ensuring representativity, we selected  $\delta=0.7$  for the second step.

Sensitivity analysis was performed on the value of  $f_F$  within the range of 0.001 to 0.1 for the first step and 0.001 to 0.006 for the second step. The calculated  $P_c(S)$  curves show that keeping the first  $f_F$  value at 0.004 enables the inclusion of a sufficient number of elements from the 2.3 $\mu\text{m}$  network for simulations to predict the higher capillary-pressures while eliminating artificial jumps in capillary-pressure.

We analysed the goodness of fit for the  $P_c(S)$  curves for the single (at 2.3 $\mu\text{m}$  and 12 $\mu\text{m}$ ), two-scale, and three-scale PNMs using the Chi-squared measure. Single-scale networks yield the poorest capillary-pressure predictions while the three-scale network and the two-scale (32.8–12 $\mu\text{m}$ ) show only minor deviations from the laboratory measurements (Figure 5). Chi-squared for the 32.8–12 $\mu\text{m}$  network is marginally better than that of the 32.8–12–2.3 $\mu\text{m}$  network,

since the Chi-squared test only compares model predictions against the laboratory measurements, but does not capture that the model does not predict capillary-pressure at low saturations for the 32.8-12 $\mu$ m combination.

Although the calculated absolute permeability values (Table 2) do not accurately match the experimental observation (50mD), the calculated values are close and within the same order of magnitude. The deviation could stem from (i) the fact that the simulations are conducted on a subsection of the acquired  $\mu$ CT images, (ii) errors introduced in noise filtering and subsequent segmentation steps, and (iii) image properties, in particular, the partial volume effect. This can cause features (e.g. pore-throats) smaller than one voxel to appear as large as a voxel in the segmented images. Larger pore-throats display less resistance to the flow and hence a higher absolute permeability is calculated.

No laboratory  $kr(S)$  measurements were available, hence simulated  $kr(S)$  curves for single and multi-scale PNMs are compared in SI. In summary, we show that the parameters involved in the network integration, as well as the number and resolution of the input single-scale networks can have a substantial impact on the shape of the  $kr(S)$  curves calculated based on the multi-scale PNMs. Future studies could aim to compare the calculated  $kr(S)$  curves with laboratory measurements to establish the effect of network integration on predicting  $kr(S)$  curves.

#### **4. Multi-scale Network Generation Workflow**

Figure 6 is a practical guide for selection of length-scales for generating a multi-scale PNM from  $\mu$ CT data and is additionally informed by thin-section imaging and MICP techniques. This information assists sample size selection, the choice of length-scales, and resolutions for multi-scale network generation.

## 5. Summary and Conclusions

A network integration approach introduced by *Jiang et al.* [2013] is used to generate representative models for a dolomite with multi-scale porosity. PNMs extracted from  $\mu$ CT images acquired at different length-scales are integrated into single multi-scale PNMs incorporating all the porosity features that exist in the rock. The main contribution of this paper is to present a workflow for effective selection of appropriate length-scales for generation of the multi-scale network. The choice of images to be combined is informed by MICP throat-size distributions. Additionally, there are two free parameters ( $\delta$  and  $f_F$ ) in the model. The integrated networks are used to reproduce  $P_c(S)$  curves, evaluated against MICP laboratory measurements. We demonstrate that  $P_c(S)$  curves calculated based on the two-scale and three-scale PNMs provide significantly closer comparisons to the laboratory measurements compared to a single-scale network model. Future studies need to validate calculated  $kr(S)$  curves against experimental measurements to optimise multi-scale network generation for predictions of multiphase fluid behaviour.

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#### Nomenclature Table:

$S$	saturation
$S^*$	the saturation at which the jump occurs
$S_{air}$	air saturation
$f_F$	Fraction of fine network
$\delta$	Nesting-domain fraction
$P_c(S)$	relative permeability
$k_r(S)$	relative permeability
$k_{rnw}(S)$	non-wetting phase relative permeability
$k_{rw}(S)$	wetting phase relative permeability
$k_{abs}$	absolute permeability
$r$	radius
$\chi^2$	Chi-squared

#### Tables:

**Table 1: Network parameters for PNM shown in Figure S3.**

Image Resolution ( $\mu\text{m}$ ), corrected for spot size	Voxel Size ( $\mu\text{m}$ )	Domain Dimensions (voxels)	Number of Nodes	Number of Bonds	Connected Porosity %	Total imaged Porosity %	$k_{abs}$ (mD)
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32.8	32	881×901×901	10318	12736	0	3.52	0
21	21	821×860×720	19897	24093	0	6.03	0
12	5	500×500×500	3418	4127	6.15	9.23	75.63
2.3	2	570×450×380	1733	2089	12.72	14.32	99.75

**Table 2: Network parameters for multi-scale PNMs**

Image Resolution ( $\mu\text{m}$ )	Number of Nodes	Number of Bonds	Connected Porosity %	Total Porosity %	$k_{abs}$ (mD)	Average coordination number
32.8-12-2.3	13956	22954	3.81	3.96	128.14	3.44
32.8-2.3	439131	534791	3.31	3.36	178.02	3.02
32.8-12	76916	100743	4.28	4.43	90.55	2.94

### Figure Captions:

**Figure 1:** (a) Backscattered SEM image of a polished thin-section of SD in three different magnifications, acquired at SEM facility at Heriot-Watt University (resolution  $\sim 0.7\mu\text{m}$ ). The left hand side image represents a tessellated image constructed from 400 fields of view stitched together, (b) Four  $\mu\text{CT}$  images of SD rock samples ( $D=2, 5, 25$  and  $38\text{mm}$ ) captured at respective resolutions of  $2.3, 12, 21$  and  $32.8\mu\text{m}$ . The scanned samples were not generated sequentially by cutting the same core, (c) PSD derived from the four images shown in (b) using a sphere fitting method [Jiang et al., 2007].

**Figure 2:** (a) Networks extracted from ten sub-domains with  $\delta$  ranging from  $0.1$  to  $1$  for the coarse-network (resolution  $21\mu\text{m}$ ), blue colour shows connected pink is globally disconnected elements, (b) Static properties of the sub-domain networks shown in (a), the blue box corresponds to the jump in the total porosity captured for  $\delta=0.4$  while the red box shows the locally connected cluster captured in the sub-domain with  $\delta=0.5$ , (c) Effect of fraction of fine-network ( $f_F$ ) on porosity and permeability of two-scale networks with  $\delta=0.7$  (see 3D renderings in Figure S4), and (d) Effect of nesting-domain size on the two-scale ( $21$  and  $2.3\mu\text{m}$ ,  $f_F=0.01$ )  $P_c(S)$  curves in comparison with laboratory measurements.

**Figure 3:** (a) The porosity of the sub-domains of the  $32.8\mu\text{m}$  network as a function of the domain fraction, (b) The  $P_c(S)$  curves for the combined  $32.8 - 2.3\mu\text{m}$  networks compared with the MICP laboratory measurements. The  $32.8\mu\text{m}$  network becomes sufficiently representative for  $\delta>0.6$  displaying converged porosity and  $P_c(S)$  curves.  $\delta$ : Nesting-domain fraction,  $f_F$ : Fraction of fine-network.

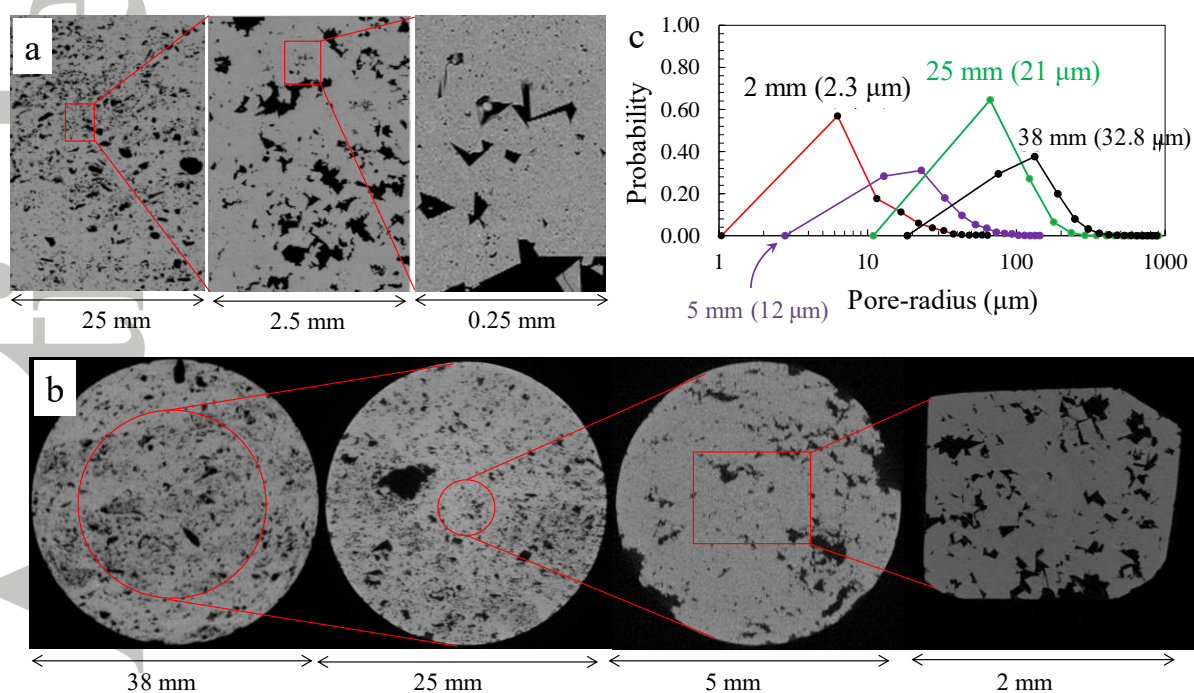
**Figure 4: The  $P_c(S)$  curves for the two-scale 32.8–12 $\mu\text{m}$  ( $\delta=0.7$ ) network for various  $f_F$ . The model predictions show a good fit to the experimental data, however, the model does not predict the higher pressure end of the curve.**

**Figure 5: The  $P_c(S)$  curves for the three-scale network compared with the laboratory data, two-scale and single-scale simulations. The plot also shows the Chi-squared ( $\chi^2$ ) measure for these networks. The three-scale network model displays the best fit to the MICP data.**

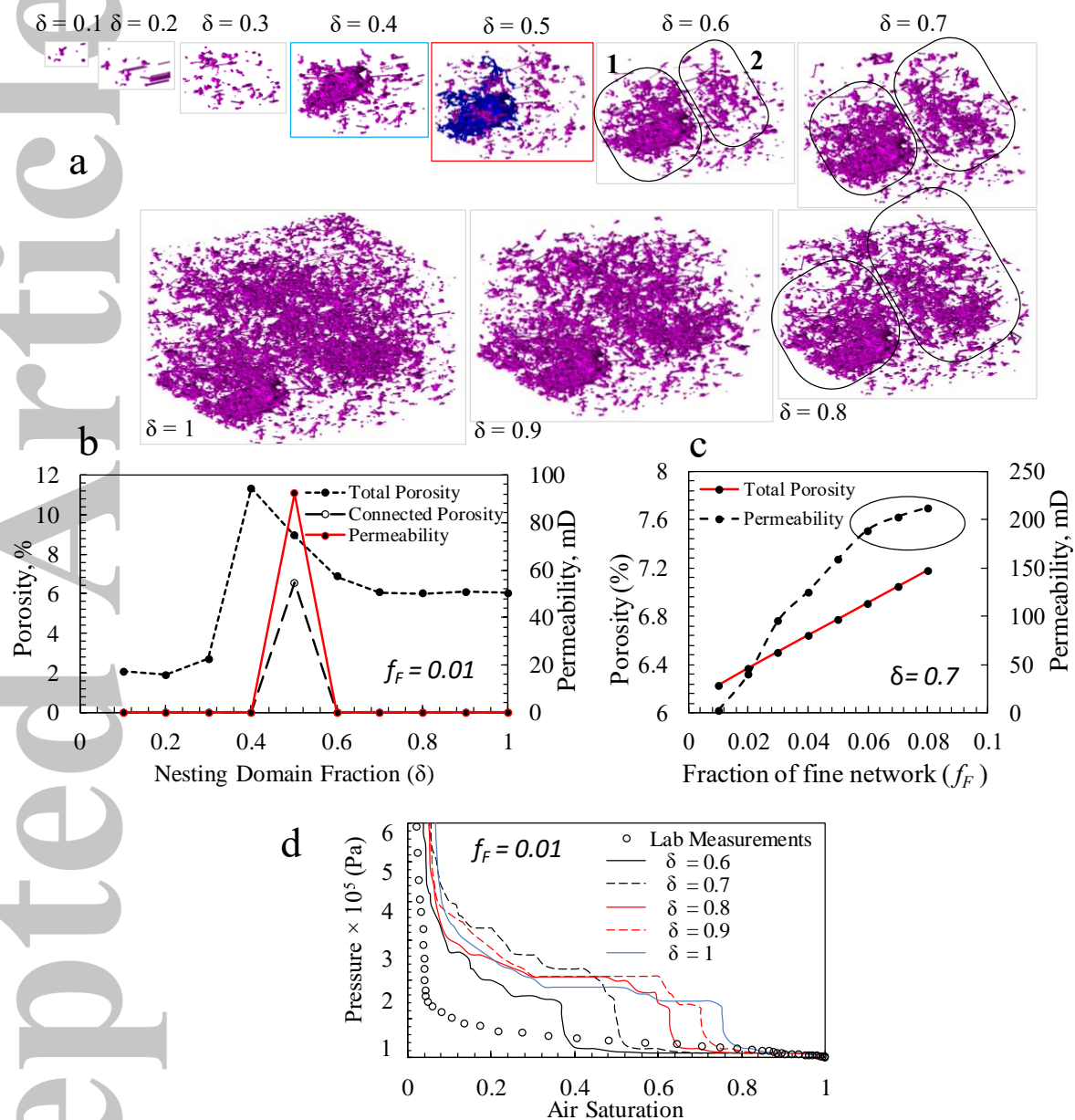
**Figure 6: Multi-scale network generation workflow and tuning.**



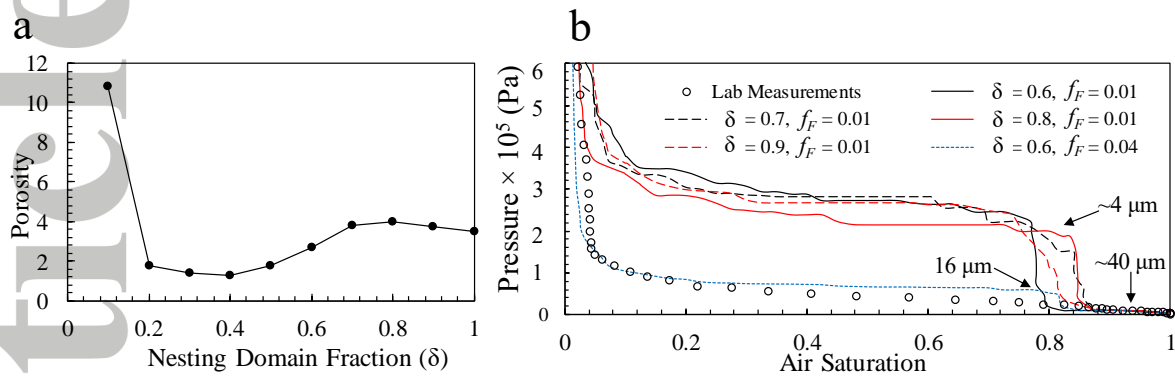




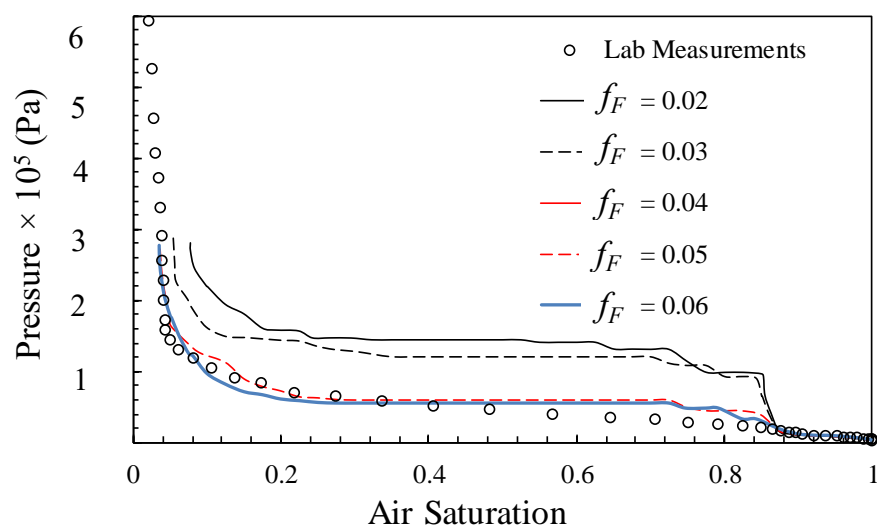






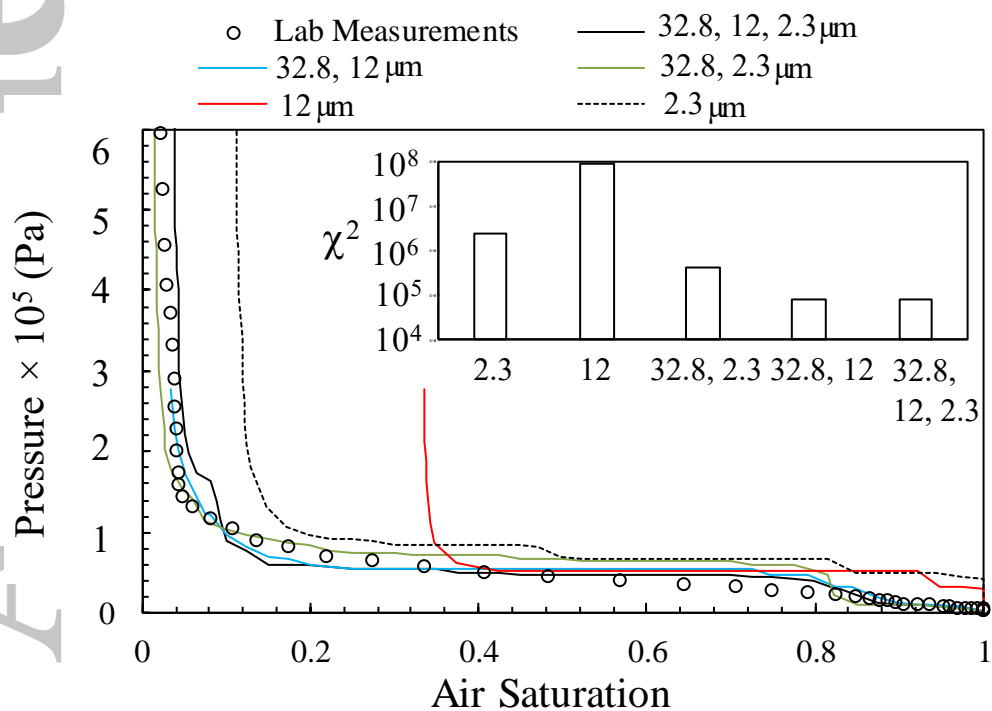










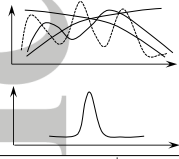




## Multi-scale Network Generation Workflow

### Does the Rock Have Multi-scale Porosity?

- High resolution thin section imaging
- Pore size distribution analysis



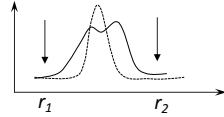
No

A single scale image with enough resolution can capture details of the pore structure.

Yes

### Pore-space Connectivity Analysis

- Take the largest plug that MICP instrument can take ( $D \sim 1$  inch), run MICP
- Plot the pore-throat size distribution



- Measure the total, effective and isolated rock porosity.

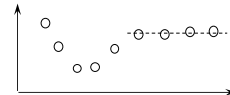
### Sample Size Selection

Take a minimum of two samples from the rock such that  $\mu$ CT images can be captured with  $r_1$  and  $r_2$  resolutions, to represent coarse and fine porosity.

Pore network extraction from each scale

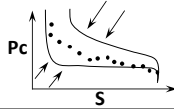
### REV Analysis

Sensitivity on the nesting domain size: Analyse properties ( $\phi$ ,  $k_{abs}$ ,  $P_c(S)$ ) of ten sub-domains of the coarse network with  $\delta = 0.1$  to 1.



### Multi-scale Network Generation

Tune the fraction of fine network ( $f_F$ ) to match the experimental  $P_c(S)$  curve as close as practically possible.



Yes

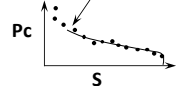
Properties converged?

No

Scan a larger sample to capture at least one REV

Does the Calculated Pc-Sat Curve match the Laboratory Data?

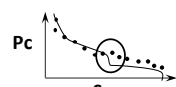
No



Yes

The rock has smaller pores that are not represented by this network.

A higher resolution image is required for the fine network.



Yes

Under-representation of a range middle size pores insufficient overlap range.

A third, middle-scale network is required.

Proceed to Relative Permeability Calculations and Other Pore-network Flow Simulations